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Scalability of the CTH Hydrodynamics Code on the Sun HPC 10000 Architecture

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Abstract

This report presents an overview of an explicit message-passing paradigm for an Eulerian finite volume method for modeling solid dynamics problems involving shock wave propagation, multiple materials, and large deformations. Three-dimensional simulations of high velocity impact were conducted on the Sun HPC 10000 computer system. The scalability of the message-passing code on this symmetrical multiple processor architecture is presented and is compared to the ideal linear multiple processor performance. The computed results are also compared to experimental data for the purpose of validating the shock physics application on the Sun HPC 10000 system.

ACKNOWLEDGMENTS

The high performance computing resources used in this study were provided by the U.S. Army Research Laboratory (ARL) Major Shared Resource Center (MSRC), operated under the auspices of the Department of Defense high performance computing modernization program. Thomas Kendall and Kathy Smith of the ARL MSRC provided timely and effective support of the subject resources, listening to suggestions and making system configuration changes on short notice in an effort to maximize performance. The efforts of these individuals and the entire ARL MSRC staff are appreciated.

The CTH hydrodynamics code is developed and maintained by the Sandia National Laboratories. The CTH project lead, Dr. Gene Hertel, provided early guidance in the development of the simulation used for the scalability testing and insight into the performance testing approach used at Sandia. This dialogue provided a solid foundation for the work described in this report.

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TABLE OF CONTENTS

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LIST OF FIGURES

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1. INTRODUCTION

The mechanics of penetration and perforation of solids have long been of interest for military applications in terminal ballistics. Kinetic energy penetration phenomena are also germane to applications involving high-mass and high-velocity debris attributable to accidents or high-rate energy release, the transportation safety of hazardous materials, the safety of nuclear reactor containment vessels, the design of lightweight body armors, the erosion and fracture of solids because of repeated impacts by liquid or solid particles, and the protection of spacecraft from meteoroid impact. A thorough review of the fundamentals of penetration and perforation and their application to practical problems has been prepared by Goldsmith (1960), Johnson (1972), Backman and Goldsmith (1978), and Zukas et al. (1982, 1990).

Analytical approaches to penetration mechanics tend to fall into three categories: empirical or quasi-analytical, approximate analytical, and numerical methods. While empirical and approximate analytical methods are quite useful for developing an appreciation of the dominant physical phenomena, they are limited in scope. Numerical methods provide a complete description of the dynamics of impacting solids, which account for the geometry of the interacting bodies; elastic, plastic and shock wave propagation; hydrodynamic flow; finite strains and deformations; high strain rate material behavior; and the initiation and propagation of failure in the colliding bodies. Computer codes for modeling wave propagation and impact have matured considerably since their initial development about 45 years ago. Today they serve as valuable tools in studies of materials and structures subjected to intense impulsive loading. Benson (1992) recently documented a comprehensive review of the physics and numerics in wave propagation codes.

Three-dimensional (3-D) simulations of high-velocity impact phenomena continue to delineate the high performance computing resources for Army applications in terminal ballistics. Current applications in high-velocity impact phenomena require the simulation time to increase from the microsecond to millisecond regime, and complex geometries dictate a finer mesh resolution which mandates a smaller time integration increment to satisfy stability criteria and additional time integration cycles. For a given Eulerian computational domain, memory requirements scale inversely with the cube of the zone size and processor requirements scale to the fourth power as the mesh is refined with smaller zones. These factors, when coupled with the requirement to model larger physical domains, are strong stimuli for exploiting scalable architectures and algorithms.

Under the aegis of the Department of Defense (DoD) high performance computing (HPC) modernization program (Jones 1996), DoD researchers are afforded access to scalable HPC resources. The successful use of scalable architectures for large-scale simulations of high-velocity impact requires reliable and robust scalable applications algorithms. The common HPC software support initiative (CHSSI) component of the DoD HPC modernization program addresses the development, validation, and demonstration of scalable software in a number of defense computational technology areas. This report presents an overview of an explicit message-passing paradigm for applications in shock physics. Scalable performance of a 3-D oblique rod impact are presented for the Sun HPC 10000 system, a new symmetric multiple processor (SMP) architecture.

2. SCALABLE PARADIGM FOR IMPACT PROBLEMS

CTH (McGlaun & Thompson 1990) is an Eulerian finite volume code for modeling solid dynamics problems involving shock wave propagation, multiple materials, and large deformations in one, two, and three dimensions. CTH is widely used across the defense research and development community to model problems in shock wave propagation. CTH employs a two-step solution scheme - a Lagrangian step followed by a remap step. The conservation equations are replaced by explicit finite volume equations that are solved in the Lagrangian step. The remap step uses operator splitting techniques to replace multi-dimensional equations with a set of one dimensional equations. The remap or advection step is based on a second order accurate method by van Leer (1977). To minimize material dispersion, several high resolution material interface trackers are available. Both analytical and tabular equations of state are available to model the hydrodynamic behavior of materials. Models for elastic-plastic behavior and high explosive detonation are also available.

Robinson et al. (1992) developed the algorithmic framework for conducting scalable Eulerian finite volume simulations for modeling problems in solid dynamics, based on object-oriented programming. Robinson demonstrated that the structured mesh of the Eulerian finite volume method is well suited for scalable paradigms employing message passing between computational sub-domains.

Scalable computer architectures are characterized by a large number of computational nodes consisting of memory, one or more commodity processors, and an internal communications network. One computing technique that can be employed on this type of architecture is referred to as single program multiple data (SPMD). Under the SPMD paradigm, the same executable code runs on each computational node, but each executable works on a different set of data. Algorithms that depend on a fixed, logically connected mesh are readily adapted to the SPMD paradigm. The technique used for SPMD parallelism in CTH is similar to the formulation developed by Robinson et al. (1992) in that the entire problem domain is divided into sub-domains that reside on individual computational nodes.

The use of "ghost" cells is a common technique for applying boundary conditions to finite difference and finite volume schemes, making the internal differencing computations independent of edges and corners in the Eulerian mesh. To adapt CTH to the SPMD paradigm, these ghost cells are used for passing messages between nodes. This practice of explicit message passing between sub-domains allows each of the individual sub-domains to have access to its neighboring sub-domains' boundary cell data. Where a sub-domain boundary is an external boundary of the overall computational domain, the ghost cell data are based on the appropriate boundary condition approximation. A simple example of this approach to mesh decomposition with explicit message passing is provided in Figure 1. A thorough description of the distributed finite volume algorithm and message communication between sub-domains is provided by Kimsey et al. (1998).

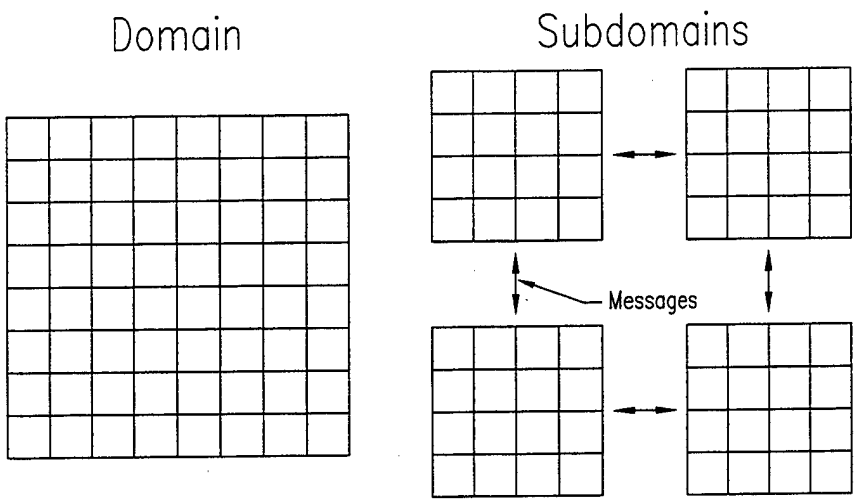

Figure 1. CTH Mesh Decomposition With Explicit Message Passing

3. SUN HPC 10000 SYSTEM

The scalability and performance trials described in this report focus on a relatively new entry into the HPC arena. The Sun HPC 10000 architecture is a unified memory access (UMA) symmetric multi-processor. It can hold as many as 64 UltraSPARC processors and 64 gigabytes (GB) of main memory. The system uses a crossbar interconnect for inter-processor communication and has an overall system bandwidth of 12.8 GB/s with memory latencies of 400 to 600 ns (Sun Microsystems 1997). The UMA architecture is designed so that any processor may access data in any segment of memory in the same amount of time, regardless of the relative locations of the processor and segment of memory in question.

The scalability study was performed with a set of HPC 10000 systems operated by the U.S. Army Research Laboratory (ARL) Major Shared Resource Center (MSRC). As of this writing, the MSRC has three systems available to support unclassified processing for defense science and technology programs. Two of these systems each have 64 processors and 64 GB of main memory. The third system has 32 processors and 32 GB of main memory. All the systems are equipped with UltraSPARC processors operating at a clock speed of 400 MHz.

Each of the systems contains several high-speed network interfaces. One of these, the asynchronous transfer mode (ATM) interface, has a peak bandwidth of 622 Mb/s and was used in trials in which the simulations were distributed across two of the three systems. The message-passing interface (MPI) (Gropp et al. 1994) was used for explicit message passing between processes (Snir et al. 1995; Sun Microsystems November 1997).

4. SCALABLE HIGH-VELOCITY IMPACT SIMULATIONS

CTH with explicit message passing has been used to model a long rod projectile impacting an oblique steel plate on the Sun HPC 10000 architecture. This problem was selected

because of well-characterized experimental data (Fugelso & Taylor 1978) and previous serial CTH simulations conducted by Hertel (1992). Fugelso and Taylor conducted a series of ballistic experiments to evaluate the effects of combined obliquity and yaw on high-density long rod projectiles. Depleted uranium (DU) alloy long rod projectiles with little or no yaw were launched into an oblique, rolled homogeneous armor (RHA) plate that had been accelerated by an explosive charge, resulting in a yawed impact in the plate frame of reference. The DU alloy (DU 0.75%Ti) projectiles were right circular cylinders with a hemisperical nose, and the impact velocities ranged from 0.85 to 1.65 km/s. Yaw and obliquity angles ranged from 0 to 70° and 10 to 0°, respectively, in the test series. The length and diameter of the projectile in Shot 58 of the test series are 7.67 cm and 0.767 cm, respectively, for a length-to-diameter ratio (L/D) of 10. The striking velocity was 1.289 km/s and the thickness of the RHA was 6.4 mm. In the laboratory frame of reference, the angle of obliquity was 73.5°, the plate velocity was 0.217 km/s, and the projectile velocity was 1.21 km/s. In the plate frame of reference, the angle of obliquity was 64.2°, the projectile velocity was 1.289 km/s, and the yaw angle was -9.3°. A schematic of the initial conditions for Shot 58 is illustrated in Figure 2.

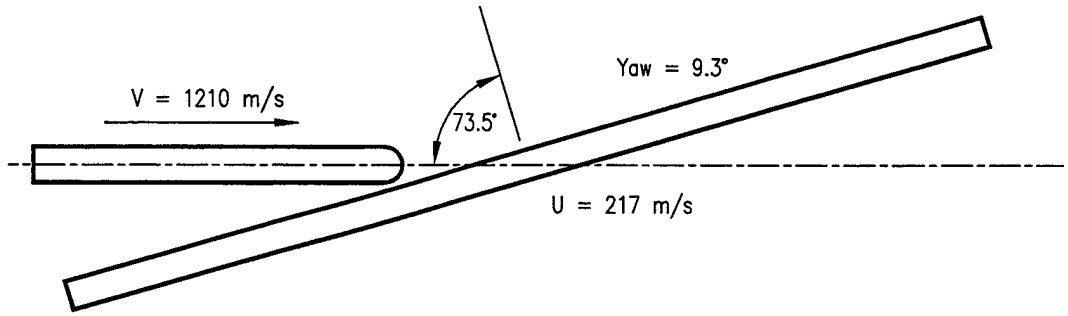

Figure 2. Initial Conditions for Combined Yaw and Obliquity Impact Simulation

The scalability study was conducted with a constant workload (i.e., number of computational cells on each processor for each of the simulations). This was done to keep the computation-to-communication ratio constant for simulations involving different numbers of processors. Maintaining a constant computation-to-communication ratio and eliminating disk access for intermediate plot and restart files during the time integration permitted the computational performance to be isolated and measured as a function of the number of processors used.

The single-processor baseline calculation used a Cartesian computational domain spanning 21.5 cm in the X direction, 3.0 cm in the Y direction, and 6.0 cm in the Z direction. The computational domain was discretized into uniform cubic zones 1 mm long, resulting in a 3-D grid of 215 by 30 by 60. As the number of processors in a simulation increased, the number of zones in the model increased accordingly to maintain a nearly constant number of computational zones per processor.

All calculations were conducted for a simulated time of 40 μs. The grid was incrementally refined by uniformly decreasing the characteristic zone length in each coordinate direction by a factor of $2^{-1/3}$. This approach doubles the total number of grid points with each

successive mesh refinement. The characteristics of the grids used in the scalability study are summarized in Table 1. In this table, the columns NI, NJ, and NK refer to the number of Eulerian cells in the x, y, and z directions, respectively, and do not include ghost cells. An alternative to this mesh refinement technique would be to double the number of zones in one direction for one refinement, then double the number of zones in another direction for the next refinement, and so on. This approach would reduce the time step by a factor of two on the first refinement and would double the number of time integration cycles (i.e., computational cycles) to reach the desired simulation time of 40 μs. The method of uniform zone size reduction resulted in a reduction of the time step by a factor of $2^{-1/3}$ with each refinement. As a result, the number of computational cycles required to reach 40 μs of simulated time increased only by a factor of approximately $2^{1/3}$ each time the number of processors doubled.

Table 1. Computational Grids Used in Scalability Study

Number of Processors	NI	NJ	NK	Total Number of Zones	Average Zones per Processor	Zone Length (mm)
1	215	30	60	387,000	387,000	1.00
2	271	38	75	772,350	386,175	0.80
4	341	48	95	1,554,960	388,740	0.63
8	430	60	120	3,096,000	387,000	0.50
16	541	76	151	6,208,516	388,032	0.40
32	683	95	191	12,393,035	387,282	0.31
48	781	109	218	18,558,122	386,628	0.28
64	860	120	240	24,768,000	387,000	0.25
96	985	137	278	37,514,710	390,778	0.22

The scalable performance of the message-passing code is measured by the "grind time," which is the average processor time required for the code to revise all flow field variables for one computational cell in a given time increment (cycle). The grind time is expressed in units of μs/(zone cycle). In a case of ideal scalability, the grind time will decrease by a factor of two for every doubling of processors used if the ratio of computation to communication is held constant.

5. SCALABILITY RESULTS

Three sets of calculations were performed to assess the scalable performance of the Sun HPC 10000 system. The first set of calculations was run on one of the 64-processor systems at the ARL MSRC. These calculations were performed with the processor and problem size combinations described in Table 1. The results of this set of simulations are represented by the square symbols in Figure 3. Also visible in the plot are two straight lines. The first straight line is a line of ideal scalability that uses the single-processor result as its anchor point. The second straight line is like the first, except that it uses the eight-processor result

as its anchor point. The results of this first set of simulations show that the two- and four-processor calculations almost exactly match the ideal performance. The calculations using eight or more processors fall slightly off the single-processor ideal scaling line. However, comparing these results to the eight-processor ideal scaling line shows that the system scales linearly up to 48 processors. The 64-processor calculation falls slightly off the eight-processor ideal scaling line. This performance penalty is caused by contention between the operating system and the application. By using all 64 processors in the system, the application has to compete with the operating system for system resources, which results in a slight degradation in performance.

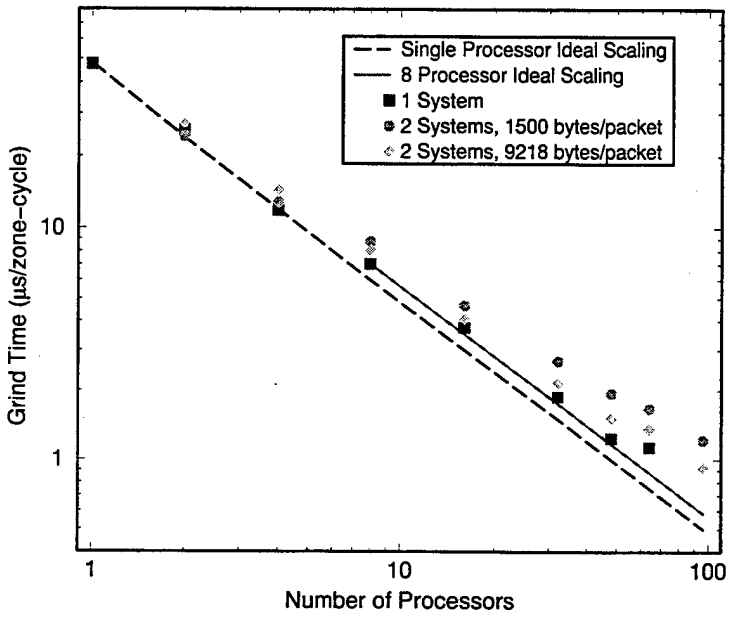

Figure 3. Ideal and Measured Scalability of CTH on the Sun HPC 10000

The shift in scalability that occurs between the four- and eight-processor results can most likely be attributed to the system processor configuration. The 64 processors reside on 16 system boards, each containing four processors and 4 GB of memory. While there is no guarantee that these two- and four-processor calculations ran on a single system board, one would expect such "on board" calculations to be the most efficient because they do not need to use the crossbar interconnect for passing data between processors. If the two- and four-processor calculations were actually run on a single system board, then the calculations using eight processors or more would all have used the crossbar interconnect for message traffic. The linear scalability observed from 8 to 48 processors shows that the crossbar interconnect was capable of handling the flow of data between processors as the problem size and number of processors used increased and that the memory access was truly symmetrical.

As stated earlier, requirements for enhanced simulation fidelity are constantly increasing. As the grid resolution is increased in explicit, finite volume simulations, the problem size and

corresponding work load increase dramatically. To solve very large problems, it is necessary to run simulations using numbers of processors that are greater than what is currently available in a single symmetric multi-processor system. To address this need, large SMP systems may be "clustered" to create a very large system for solving highly resolved problems. The second and third sets of simulations were performed to determine the scalability that could be obtained by clustering two Sun HPC 10000 systems. For these trials, the ATM interface was used for the transfer of data between the two systems. This interface has a maximum data transfer rate of 622 Mb/s.

The ATM interfaces were configured to communicate using data packets that are 1,500 bytes in size for the second set of trials. This relatively small packet size resulted in a requirement to transfer a large number of packets for large problems. The results of these simulations are represented by the circle markers in the scalability plot of Figure 3. A comparison of these markers to the square symbols for the single-system trials shows that the performance is degraded as the problem size (and number of processors) increases. For the 64-processor simulation (which uses a problem size of approximately 24.7 million Eulerian zones), the grind time increased by 47% over the same calculation run on a single system. The performance limitation in these simulations is the transfer of data between the two SMP systems through the ATM interface.

In an attempt to improve the communication performance between the two SMP systems, the ATM interface was reconfigured to use an increased packet size of 9,218 bytes. The third and final set of simulations was run using this larger packet size, and the results are represented by the diamond symbols in Figure 3. These results show a noticeable improvement in the performance for large problem sizes. For the simulation using 64 processors, the grind time was 20% greater than the single-system calculation. While the large packet results do not match those of the single-system performance, they provide a valuable initial demonstration of the ability to effectively use large, clustered SMP systems to solve problems using large numbers of processors.

The computational performance of CTH on any computer architecture is irrelevant if the results are incorrect. To verify the accuracy of the results computed on the Sun HPC 10000, the single-processor and the 48-processor simulations were extended to a simulated time of 100 μs and compared to experimental data. Data obtained from the experiment were the residual length and velocity of the rod after passing through the target plate (Hertel 1992). The initial impact conditions are provided in Figure 2. The residual rod length and velocity in the experiment were 5.55 cm and 1069 m/s, respectively. The single-processor calculation, which employed a uniform zone size of 1 mm, produced a residual rod length of 5.93 cm (6.8% greater than the experiment) and a residual velocity of 1002 m/s (6.3% lower than the experiment). The 48-processor simulation employed a uniform zone size of 0.28 mm and resulted in a residual rod length of 6.14 cm (10.6% greater than the experiment) and a residual rod velocity of 1020 m/s (4.6% lower than the experiment). Figure 4 provides an illustration of the finite plate perforation at 100 μs for both calculations. The upper left side of each image shows the target plate after it was perforated by the penetrator. The simulation was set up with the rod impacting the middle of the plate. As a result, the calculation used a plane of symmetry about the point of impact. In the figure, the rod

geometry is reflected about the plane of symmetry to provide a detailed view of the deformed penetrator after impact.

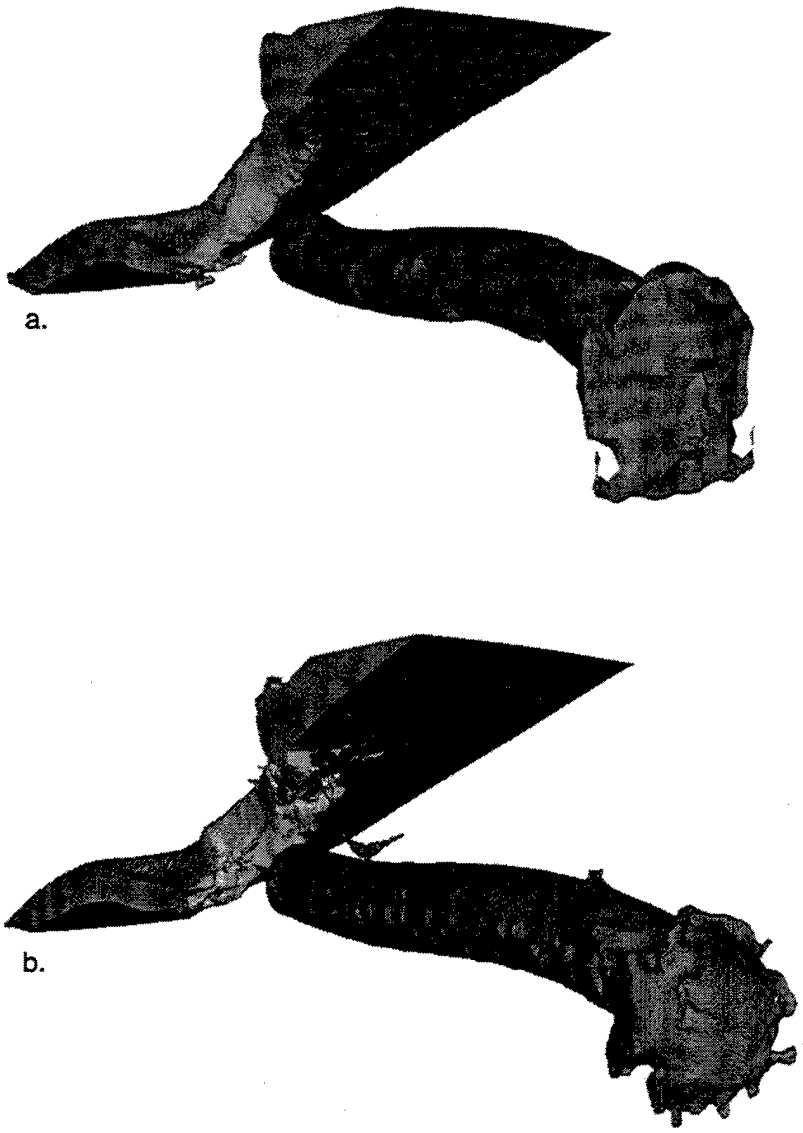

Figure 4. Finite Plate Perforation at 100 μs: a. 1-mm Zones, b. 0.28-mm Zones

6. SUMMARY

In a previous effort, the CTH hydrodynamics code was adapted to an SPMD programming paradigm to exploit large, scalable computer architectures. This paradigm involves the decomposition of the structured mesh into computational sub-domains, with explicit message passing used to communicate data between the multiple processes used in solving the problem. This method has been demonstrated to scale linearly as the number of processors and corresponding problem size increased.

A new system architecture in the HPC arena is the Sun HPC 10000 system. A series of numerical simulations was performed to assess the scalability of CTH on this system. Three sets of trials were performed. The first set was limited to a single system containing 64 processors. The study demonstrated that the application scales linearly on this system to 48 processors. However, the performance of the application on 64 processors suffered a slight performance degradation as a result of contention with the operating system.

Two additional sets of simulations were run to assess the scalability of large, clustered SMP systems to solve large problems using large numbers of processors. Data communication between SMP systems for these trials used packet sizes of 1,500 bytes and 9,218 bytes. The 1,500-byte/packet trials suffered a noticeable performance degradation as the problem size and resulting message traffic increased. Tests using the larger packet size showed a significant improvement in performance for the large problems. While the performance in these simulations did not match that of the single-system simulations, these trials demonstrated the ability to cluster large SMP systems to solve very large problems.

The results described in this report do not provide enough information to determine whether these results will continue to scale for large groups of SMP systems. Additional trials with at least four SMP systems would provide a better indication of the ability to use large SMP systems for this purpose. While the two sets of multiple system sets show an improvement in performance with increased packet size, this configuration is by no means optimal. Additional work is needed to determine the best type of dedicated network configuration to use for building a cluster of this particular system for solving very large problems.

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This report presents an overview of an explicit message-passing paradigm for an Eulerian finite volume method for modeling solid dynamics problems involving shock wave propagation, multiple materials, and large deformations. Three-dimensional simulations of high velocity impact were conducted on the Sun HPC 10000 computer system. The scalability of the message-passing code on this symmetrical multiple processor architecture is presented and is compared to the ideal linear multiple processor performance. The computed results are also compared to experimental data for the purpose of validating the shock physics application on the Sun HPC 10000 system.

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